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Smoothed polygonal finite element method for generalized elastic solids subjected to torsion

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ABSTRACT

Orthopaedic implants made of titanium alloy such as Ti-30Nb-10Ta-5Zr (TNTZ-30) are biocompatible and exhibit nonlinear elastic behavior in the 'small' strain regime (Hao et al., 2005). Conventional material modeling approach based on Cauchy or Green elasticity, upon linearization of the strain, inexorably leads to Hooke's law which is incapable of describing the said nonlinear response. Recently, Rajagopal introduced a generalization of the theory of elastic materials (Rajagopal, 2003, 2014), wherein the linearized strain can be expressed as a nonlinear function of stress. Consequently, Devendiran et al. (2016) developed a thermodynamically consistent constitutive equation for the generalized elastic solid, in order to capture the response of materials showing nonlinear behavior in the small strain regime. In this paper, we study the response of a long cylinder made of TNTZ-30 with non-circular cross section subjected to end torsion. An explicit form of the constitutive equation derived in Devendiran et al. (2016) is used to study the response of the cylinder. The cross-section is discretized with quadratic serendipity polygonal elements. A novel one point integration rule is presented to compute the corrected derivatives, which are then used to compute the terms in the stiffness matrix. Unlike the conventional Hooke's law, the results computed using the new constitutive equation show stress softening behavior even in the small strain regime.

1. Introduction

Presently, the orthopaedic implants are made of stainless steel and alloys of cobalt and titanium such as Co-Cr and Ti-6Al-4V. Vanadium present in Ti-6Al-4V is known to be toxic to the human body and the present effort is to find a more biocompatible titanium alloy using non-toxic elements such as Nb, Ta and Zr. The Young's modulus of the alloys that are currently in use are much higher than that of the cortical bone, the bone's being in the range of 10–30 GPa [5]. The implants made of such alloys tend to support a larger stress in comparison to the bone resulting in bone atrophy [6], which eventually leads to the loosening of screws fastening the implants. Therefore, it is imperative that the modulus of the implant matches that of the bone. Recently developed non-toxic titanium alloys such as Ti-30Nb-12Zr [7], Ti-24Nb-4Zr-7.9Sn [1], Ti-29Nb-13Ta-4.6Zr [8] and Ti-30Nb-(8-10) Ta-5Zr [9] approaches the modulus of the cortical bone and have good fatigue life. Sakaguch [10] studied the effect of the amount of Nb(Niobium) in TNTZ alloy on the mechanical properties. For a 30% Nb content, the cyclic tensile loading showed nonlinear elastic behavior up to 2% strain, the deviation from linearity beginning at strains as small as 0.005. Interestingly, the other alloys of TNTZ undergoes deformation induced martensitic phase transformation, which result in permanent deformation, but the TNTZ-30 alloy undergoes pure lattice distortion until 2% strain.

Linearization of classical theories of elasticity, namely Green or Cauchy elasticity only leads to Hooke's law, which is incapable of describing the nonlinear response exhibited at 'small' strain levels. Further, empirical models such as Ramberg-Osgood equation, while it can describe the uniaxial nonlinear elastic behavior of TNTZ-30 at small strain levels, cannot be used to describe the mechanical response for a more complex boundary condition. In order to alleviate such a shortcoming, Rajagopal et al. [2] introduced a generalized class of elastic material, wherein an elastic material is defined as the one which does not dissipate energy. By following the seminal contribution of Rajagopal, a series of papers were published [11,3,4]. Devendiran et al. [4] obtained a general implicit constitutive equation for the generalized elastic solid in terms of the Gibbs potential involving the second Piola Kirchoff stress tensor. They also obtained a special constitutive equation wherein the linearized strain is a nonlinear function of the Cauchy stress, which accurately describes the mechanical response

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of TNTZ-30. Bustamante et al. [12] studied a class of isotropic generalized elastic solids under small deformation. The nonlinear constitutive equation predicts an increase in the gradient of strain with an increase in the stress. Ortiz et al. [13,14] have solved a few boundary value problems numerically using finite element methods for a strain limiting constitutive equation.

The conventional finite element method (FEM) was adopted in earlier studies and were restricted to simplex elements [12–14]. With advancements in mathematical software and seminal work of Wachspress [15], Sukumar and Tabarraei [16], Dasgupta [17] to name a few, and the recent drive from the computer graphics community [18–21], the discretization of domain and approximations over arbitrary polytopes is now feasible for practical applications. The use of polygonal elements (elements with more than four sides in two dimensions) relaxes the constraint on the mesh topology and has opened up a new area of finite elements called '*polygonal finite elements*'. For a comprehensive overview of the construction of approximation functions over arbitrary polytopes, interested readers are referred to [22,23], and the references therein. The major objectives of the paper are the following:

- To study the torsional behavior of non-circular shafts made of TNTZ-30, which finds applications in bio-medical implants and shows nonlinear response even in small strain regime. The explicit constitutive relation proposed in [4] is employed for this study.
- To employ polygonal finite elements for spatial discretization.[1] The conventional approaches, for example using triangular quadrature to evaluate the terms in the bilinear-linear form requires very high order quadrature rules, at least 13n integration points, where n is the number of sides of the polygon. Here, we propose a new one point integration scheme that requires only n integration per polygon. The accuracy and the convergence properties are discussed in the revised manuscript.

The nonlinear constitutive equation, the governing equations and the boundary conditions are described in Section 2. Section 3 describes the solution procedure mainly focusing on the weak formulation and the spatial discretization. We discuss the linear smoothing technique for computing the corrected derivatives along with the one point integration scheme and the Newton method in subsections 4.1 and 4.2, respectively. The implemented algorithm is described in Appendix A. In Section 5, we discuss the numerical results for a classical boundary value problem and the last section concludes the work.

2. Theoretical formulation

2.1. Kinematics

Consider an abstract body B, let $\mathbf{X} \in B$ denote the position of any point in the reference configuration $\kappa_r(B)$ and let $\mathbf{x} \in B$ be the corresponding position of the point in the current configuration $\kappa_t(B)$, given as,

$$\mathbf{x} = \chi(\mathbf{X}, t), \tag{1}$$

where, χ is the motion function which maps the points from the reference onto the current configuration. The deformation gradient is given by,

$$\mathbf{F} = \frac{\partial \chi}{\partial \mathbf{X}}, \tag{2}$$

and the displacement field $\mathbf{u}$ is given by,

$$\mathbf{u} = \mathbf{x} - \mathbf{X}. \tag{3}$$

By taking the material derivative of the displacement field, the Green strain is given by,

$$\mathbf{E} = \frac{1}{2}\left[\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}} + \nabla\mathbf{u}^{\mathrm{T}}\nabla\mathbf{u}\right], \tag{4}$$

where $\nabla\mathbf{u} = \frac{\partial \mathbf{u}}{\partial \mathbf{X}} = \mathbf{F} - \mathbf{I}$. When the strains are small i.e. $\max\|\nabla\mathbf{u}\| = \mathcal{O}(\delta)$, where $\delta \ll 1$, we can neglect the higher order terms of $\nabla\mathbf{u}$ in Eq. (4) and can write the strain in linearized form as,

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left[\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right]. \tag{5}$$

2.2. Constitutive equation

In this section, we give an overview of the constitutive equations derived within the implicit class of elasticity theory. For detailed derivation and proof, interested readers are referred to [4] and references therein. Consider a homogeneous, isotropic body undergoing homothermal process. Bustamante [24] and Bustamante and Rajagopal [12] proposed the existence of a scalar potential $W(\mathbf{T})$ for the implicit class of materials, such that,

$$\boldsymbol{\varepsilon} = \frac{\partial W(\mathbf{T})}{\partial \mathbf{T}}. \tag{6}$$

For an isotropic material $W(\mathbf{T})$ is a function of the invariants of the Cauchy stress, $\mathbf{T}$, i.e. $W(\mathrm{I}_{\mathbf{T}}, \mathrm{II}_{\mathbf{T}}, \mathrm{III}_{\mathbf{T}})$ and take the following form [4]:

$$\begin{aligned} W(\mathrm{I}_{\mathbf{T}}, \mathrm{II}_{\mathbf{T}}, \mathrm{III}_{\mathbf{T}}) = {} & \left(1 + \frac{\beta_0}{2}\right)\mathrm{tr}(\mathbf{T}) + \frac{\beta_1}{2}\mathrm{tr}(\mathbf{T}^2) \\ & - \frac{\beta_2}{\mathrm{n}\beta_3}\left(1 + \beta_3\mathrm{tr}(\mathbf{T}^2)\right)\mathrm{E}_{\left(\frac{\mathrm{n}-2}{\mathrm{n}}\right)}\left[-(1 + \beta_3\mathrm{tr}(\mathbf{T}^2))^{\mathrm{n}/2}\right], \end{aligned} \tag{7}$$

where $E_{\left(\frac{n-2}{n}\right)}$ is the exponential integral, which is defined as:

$$E_a[z] := \int_1^{\infty} \frac{\exp(-zt)}{t^a}\mathrm{d}t. \tag{8}$$

Upon substituting Eq. (7) into, Eq. (6), we have,

$$\boldsymbol{\varepsilon} = \beta_0(tr\mathbf{T})\mathbf{1} + \beta_1\mathbf{T} + \beta_2\exp\left(\left[\sqrt{1 + \beta_3\mathrm{tr}\left(\mathbf{T}^2\right)}\right]^{\mathrm{n}}\right)\mathbf{T}, \tag{9}$$

where $\beta_0, \beta_1, \beta_2$, β_3 and n are material parameters. There are restrictions on the sign of these material parameters, i.e. $(3\beta_0 + \beta_1) > 0$ and $\beta_1 > 0$, hence $\beta_0 < 0$ and $\beta_2, \beta_3, n > 0$. Here, β_2, β_3 and n are called the softening parameters as there is a reduction in the stresses, as predicted by Eq. (9), when compared with a linearized elastic model. Note that, when $\beta_2 = 0$, the above equation reduces to the generalized Hooke's law which is applicable for linear elastic solids. This is important because as we keep reducing the strain, even the nonlinear elastic material shows some linear behavior, so the constitutive equation should be able to predict the linear response as well. Also, as the strain increases within small strain regime, the exponential term of the constitutive equation becomes more dominant and this predicts the deviation from the linear response. Devendiran et al. [4] showed that Eq. (9) can also be derived from Gibbs potential, however, terms involving the product of $\mathbf{T}$ and $\boldsymbol{\varepsilon}$ should be ignored. For our analysis of stress response of the Titanium alloy, we use the explicit constitutive equation given by Eq. (9).

2.3. Governing differential equations for torsion

In this section, we derive the governing differential equations for a prismatic cylindrical member subjected to end torsion with the constitutive equation described in the previous section (Sec-

[1] Elements with arbitrary shapes provide flexibility in meshing and yields improved accuracy as evident in the literature.